

3-dodecen-1-al

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|-----------------------------|---|
| Other names: | dodec-3-en-1-al |
| Inchi: | InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h9-10,12H,2-8,11H2,1H3/b10-9+ |
| InchiKey: | HBBONAOKVLYWBI-MDZDMXLPSA-N |
| Formula: | C12H22O |
| SMILES: | CCCCCCCCC=CCC=O |
| Mol. weight [g/mol]: | 182.30 |
| CAS: | 68083-57-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 30.86 | kJ/mol | Joback Method |
| hf | -259.37 | kJ/mol | Joback Method |
| hfus | 29.33 | kJ/mol | Joback Method |
| hvap | 48.98 | kJ/mol | Joback Method |
| log10ws | -3.98 | | Crippen Method |
| logp | 3.882 | | Crippen Method |
| mcvol | 177.210 | ml/mol | McGowan Method |
| pc | 1985.89 | kPa | Joback Method |
| rinpol | 1365.00 | | NIST Webbook |
| rinpol | 1365.00 | | NIST Webbook |
| rinpol | 1359.00 | | NIST Webbook |
| ripol | 1734.00 | | NIST Webbook |
| ripol | 1734.00 | | NIST Webbook |
| tb | 526.78 | K | Joback Method |
| tc | 700.00 | K | Joback Method |
| tf | 261.92 | K | Joback Method |
| vc | 0.705 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 418.84 | J/molxK | 526.78 | Joback Method |
| cpg | 434.14 | J/molxK | 555.65 | Joback Method |
| cpg | 448.75 | J/molxK | 584.52 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 462.70 | J/molxK | 613.39 | Joback Method |
| cpg | 476.02 | J/molxK | 642.26 | Joback Method |
| cpg | 488.73 | J/molxK | 671.13 | Joback Method |
| cpg | 500.86 | J/molxK | 700.00 | Joback Method |
| dvisc | 0.0046993 | Paxs | 261.92 | Joback Method |
| dvisc | 0.0019373 | Paxs | 306.06 | Joback Method |
| dvisc | 0.0009985 | Paxs | 350.21 | Joback Method |
| dvisc | 0.0005970 | Paxs | 394.35 | Joback Method |
| dvisc | 0.0003959 | Paxs | 438.49 | Joback Method |
| dvisc | 0.0002830 | Paxs | 482.64 | Joback Method |
| dvisc | 0.0002140 | Paxs | 526.78 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C68083578&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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